Abstract for an Invited Paper
for the mar01 Meeting of
The American Physical Society

Nanoelectronic Modeling (NEMO):
Moving from commercial grade 1-D simulation to prototype 3-D simulation

GERHARD KLIMECK, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109[1]

The quantum mechanical functionality of commercially pursued heterostructure devices such as resonant tunneling diodes (RTDs), quantum well infrared photodetectors, and quantum well lasers are enabled by material variations on an atomic scale. The creation of these heterostructure devices is realized in a vast design space of material compositions, layer thicknesses and doping profiles. The full experimental exploration of this design space is unfeasible and a reliable design tool is needed. The Nanoelectronic Modeling tool (NEMO) is one of the first commercial grade attempts for such a modeling tool. NEMO was developed as a general-purpose quantum mechanics-based 1-D device design and analysis tool from 1993-97 by the Central Research Laboratory of Texas Instruments (later Raytheon Systems). NEMO enables[2] the fundamentally sound inclusion of the required[3,4] physics: bandstructure, scattering, and charge self-consistency based on the non-equilibrium Green function approach. A new class of devices which require full 3-D quantum mechanics based models is starting to emerge: quantum dots, or in general semiconductor based deca-nano devices. We are currently building a 3-D modeling tool based on NEMO to include the important physics to understand electronic stated in such superscaled structures. This presentation will overview various facets of the NEMO 1-D tool such electron transport physics in RTDs, numerical technology, software engineering and graphical user interface. The lessons learned from that work are now entering the NEMO 3-D development and first results using the NEMO 3-D prototype will be shown. More information about the publically available NEMO 1-D executables can be found at http://hpc.jpl.nasa.gov/PEP/gekco/nemo

[1]Recent work performed in collaboration with Chris Bowen (JPL) and Tim Boykin (U of Alabama Huntsville).
NEMO 1-D work with Roger Lake, Chris Bowen, Dan Blanks, Tim Boykin (UAH), Manhua Leng, Chenjing Fernando and William Frensley (Texas Instruments, later Raytheon, U. of Texas at Dallas, UAH)

[2]R. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, J. Appl. Phys. **81**, 7845 (1997).
[3]G. Klimeck *et al.*, in the *1997 55th Annual Device Research Conference Digest*, (IEEE, NJ, 1997), p. 92
[4]R. C. Bowen *et al.*, J. Appl. Phys **81**, 3207 (1997).